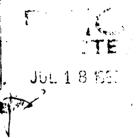


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On the Lanczos Method for Solving Symmetric Linear Systems with Several Right-Hand-Sides

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Technical Report YALEU/DCS/RR-396



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YALE UNIVERSITY DEPARTMENT OF COMPUTER SCIENCE

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Abstract

This paper analyses two methods based on the Lanczos algorithm for solving large sparse symmetric linear systems with several right hand sides. The methods examined are suitable for the case where the right sides are not too different from one another as is often the case in time dependent or parameter dependent problems. We will show in particular that a modified Lanczos algorithm, introduced by Parlett is in some sense equivalent to the block Lanczos algorithm.

On the Lanczos Method for Solving Symmetric Linear Systems with Several Right-Hand-Sides

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1. Introduction

In many applications one needs to solve several symmetric linear systems of the form

$$A x^{(i)} = b^{(i)}$$
 $i=1,2..k.$ (1)

When all of the right hand sides are available simultaneously, then several block methods can be successfully applied to (1), in particular the block Lanczos algorithm [5, 11], the block Stiefel method [11, 12].

In practice it is often the case that the $b^{(i)}$'s are not available at the same time, i.e. that a given right hand side $b^{(1)}$ depends on the solutions $x^{(i)}$, j=1,..i-1 of the previous systems. Then the block methods are no longer applicable. For this common situation, Parlett [7] suggested to use the Lanczos algorithm to solve the first system and to save the Lanczos vectors thus generated in order to provide good approximate solutions to the subsequent systems. For example, an approximate solution to the second linear system can be obtained by using a projection (Galerkin) technique onto the Krylov subspace generated when solving the first linear system. We refer to this as the Lanczos-Galerkin projection procedure. The approximation obtained from the Lanczos-Galerkin projection process alone may not be sufficiently accurate and a further refinement is often needed. A suitable and efficient way of improving the Lanczos-Galerkin approximate solution is to use a special Lanczos process introduced by Parlett [7] which consists of orthogonalizing the current Lanczos vector not only against the previous two vectors, as is classically done, but also against the Lanczos vector of the previous Krylov subspace. We will refer to this technique as the modified Lanczos algorithm.

The purpose of the present paper is to analyse these techniques, from the theoretical point of view. We will establish an error bound which will show that the Lanczos-Galerkin procedure will provide a good accuracy under the condition that the residual vector of the new system is almost contained in the previously generated Krylov subspace. We will also show that the modified Lanczos algorithm is, in a certain sense, equivalent to a block-Lanczos method with a particular initial system.

We will start by a brief presentation of the Galerkin projection methods based on the Lanczos algorithm as described in [7]. Then we will analyse the techniques from a theoretical point of view and give a priori error bounds for the Lanczos-Galerkin method. Finally we will show the relation with the block Lanczos method.

2. The Lancsos algorithm for solving a linear system

In this section we briefly describe the Lanczos method for solving linear systems. Consider the (single) linear system:

$$A x = b (2)$$

Suppose that a guess x_0 to the solution is available and let r_0 be its residual vector $r_0 = b-Ax_0$. Then the Lanczos algorithm for solving (2) can be described as follows:

Algorithm:

Stage 1: Generate the Lanczos Vectors

- Start: $v_1 = r_0/(\beta := ||r_0||)$
- For j=1,2..m do:

Compute:

$$\boldsymbol{\alpha}_{\mathbf{j}} := (\mathbf{A}\mathbf{v}_{\mathbf{j}}, \mathbf{v}_{\mathbf{j}}) \tag{3}$$

$$\hat{\mathbf{v}}_{i+1} := \mathbf{A}\mathbf{v}_i - \alpha_i \mathbf{v}_i - \beta_i \mathbf{v}_{i-1} , \qquad (\beta_1 \mathbf{v}_0 = 0)$$

$$\beta_{i+1} := ||\hat{\mathbf{v}}_{i+1}|| \tag{5}$$

$$\mathbf{v}_{i+1} := \hat{\mathbf{v}}_{i+1} / \beta_{i+1} \tag{6}$$

Stage 2: Form the approximate solution

$$x_{m} := x_{0} + V_{m} T_{m}^{-1} (\beta e_{1})$$
 (7)

where $V_m = [v_1, v_2, ... v_m]$ and T_m is the tridiagonal matrix:

In theory, the vectors \mathbf{v}_i computed from this process form an orthonormal basis of the Krylov subspace $K_m = \operatorname{span}\{r_0, Ar_0, ...A^{m-1}r_0\}$. If we denote by V_m the matrix $V_m = [v_1, ...v_m]$ then we have $V_m^T A V_m = T_m$ which means that T_m is nothing but the matrix representation of the section of A in the Krylov subpace K_m with respect to the basis V_m . Furthermore, it is easily seen that

the Lanczos algorithm realizes a projection process, i.e. a Galerkin process, onto the Krylov subspace K_m , see e.g. [7, 9]. In other words the approximate solution x_m can be found by expressing that it belongs to the affine subspace $x_0 + K_m$ and that its residual vector b- Ax_m is orthogonal to K_m . Denoting by P_m the orthogonal projector onto K_m , this means that the Lanczos method solves the approximate problem:

Find
$$x_m \in x_0 + K_m$$
 such that:

$$P_{m}(b-Ax_{m})=0 (9)$$

The approximation thus computed is identical with that provided by m steps of the conjugate gradient (CG) method when A is positive definite [7]. When A is not positive definite this relation between the Lanczos algorithm and the CG method can be exploited to derive stable generalizations of the CG algorithm to symmetric indefinite systems [6, 7, 2, 10].

A well known and troublesome misbehavior of the Lanczos algorithm is the loss of orthogonality of the v_i's. Fortunately, this does not prevent the method from converging but often results in an important slow down. Parlett [7] and Simon [13] have made the important observation that the fast convergence properties can be regained by resorting to different sorts of partial reorthogonalizations. This important matter will be further discussed in the last section.

3. The Lanczos-Galerkin projection method

Consider now the two linear systems

$$A x^{(i)} = b^{(i)}$$
 $i=1,2$ (10)

and assume that m steps of the Lanczos algorithm described in the previous section have been performed to solve the first system in a first pass. We would like to use the information gathered during the solution of the first system to provide an approximation to the second system:

$$A x^{(2)} = b^{(2)}. (11)$$

Clearly, we assume that the vectors v_i , i=1,2...m as well as the tridiagonal matrix (8) have been saved, possibly in some secondary storage.

Suppose that we have an initial guess $x_0^{(2)}$ to the solution of (11). Let $r_0^{(2)}$ be the residual vector of $x_0^{(2)}$, that is, $r_0^{(2)} = b^{(2)} - Ax_0^{(2)}$. A natural way of improving the approximation $x_0^{(2)}$ is by means of the Galerkin method onto the Krylov subspace K_m generated for the solution of the first system. This will yield an approximate solution \bar{z} defined by:

$$\bar{z} = x_0^{(2)} + V_m T_m^{-1} V_m^T r_0^{(2)} = x_0^{(2)} + \bar{y}$$
 (12)

which is obtained by solving the m-dimensional problem:

$$P_m(b^{(2)} - Az) = 0$$

or equivalently

$$V_{m}^{T}(b^{(2)} - Az) = 0 (13)$$

for z belonging to the affine subspace $x_0^{(2)} + K_m$. We will refer to the above method as the Lanczos-Galerkin process.

One important question concerning the approximation obtained from the above Lanczos-Galerkin process is its accuracy. Let us first recall that when A is positive definite we can define the A^{-1} -norm of a vector as $||u||_{A^{-1}} = (A^{-1}x,x)^{1/2}$ and that the projection process described above minimizes the A^{-1} -norm of the residual vector over all vectors of the form $x_0^{(2)} + y$ where y belongs to K_m [4]. In the following we denote by P_m the orthogonal projector onto K_m , where K_m is the Krylov subspace obtained from m steps of the Lanczos algorithm for solving the first system.

Proposition 1: Assume that A is symmetric positive definite with largest eigenvalue λ_1 and smallest eigenvalue λ_N . Then the approximation \bar{z} obtained from the Lanczos Galerkin projection process (12) is such that

$$||b^{(2)} - A \bar{z}||_{A^{-1}} = ||(I - P_m)r^{(2)}||_{A^{-1}} + \epsilon$$
(14)

where

$$|\epsilon| \le \frac{|\alpha|}{T_{-}(\gamma)} \tag{15}$$

in which $\gamma = (\lambda_1 + \lambda_N) / (\lambda_1 - \lambda_N)$, α is the first component of $P_m r_0^{(2)}$ in the basis $\{v_1, Av_1, ..., A^{m-1}v_1\}$ and T_m represents the Chebyshev polynomial of degree m of the first kind.

Proof: The residual vector $\bar{r} = b^{(2)} - A \bar{z}$ is such that

$$\bar{r} = b - A(x_0^{(2)} + \bar{y})$$

= $r_0^{(2)} - A \bar{y}$

where \bar{y} is the vector of K_m computed from equation (12). The residual \bar{r} can be further decomposed as:

$$\bar{\mathbf{r}} = (P_m \mathbf{r}_0^{(2)} - A\bar{\mathbf{y}}) + (I - P_m) \mathbf{r}_0^{(2)}$$
 (16)

Clearly, the projection method (12) also solves the system A $y = P_m r_0^{(2)}$ by the same Galerkin

process. Hence the vector \bar{y} also minimizes $\|P_m r_0^{(2)} - Ay\|_{A^{-1}}$ over all vectors y of K_m . Next, from (16) we have by the second triangle inequality:

$$|||\bar{r}||_{A^{-1}} - ||(I-P_m)r_0^{(2)}||_{A^{-1}}| \le ||P_mr_0^{(2)} - A\bar{y}||_{A^{-1}}$$
(17)

Let us set $\epsilon(y) = ||P_m r_0^{(2)} - Ay||_{A^{-1}}$, and write $P_m r_0^{(2)}$ as $P_m r_0^{(2)} = q(A)v_1$ where q is a polynomial of degree not exceeding m-1. Clearly, the scalar α defined in the proposition is the constant term in the polynomial q, i.e. $\alpha = q(0)$. Since \bar{y} minimizes $\epsilon(y)$ for $y \in K_m$, if we write $y = s(A)v_1$, and define the polynomial $p(\lambda) = q(\lambda) - \lambda s(\lambda)$, we see that

$$|| P_{m} r_{0}^{(2)} - A \bar{y} ||_{A^{-1}} = \min_{p \in P_{m,1}, p(0) = \sigma} || p(A) v_{1} ||_{A^{-1}}$$
(18)

where P_{m-1} represents the set of all polynomials p of degree $\leq m-1$. The above equality can be rewritten as:

$$\|P_{\mathbf{m}}\mathbf{r}_{0}^{(2)} - A \bar{\mathbf{y}}\|_{A^{-1}} = \|\alpha\| \min_{\mathbf{p} \in P_{\mathbf{m},1}, \mathbf{p}(0)=1} \|\mathbf{p}(A)\mathbf{v}_{1}\|_{A^{-1}}$$

The last term of the right hand side is a classical factor in the theory of the conjugate gradient method and a well-known upper bound for it is available (e.g. [2]) and yields

$$||P_{m}r_{0}^{(2)} - A \overline{y}||_{A^{-1}} \leq |\alpha| \frac{1}{T_{m}(\gamma)}$$
with $\gamma = (\lambda_{1} + \lambda_{N})/(\lambda_{1} - \lambda_{N})$.

The result finally follows from inequality (19) and inequality (17)

Let us now interpret the result of the proposition. Notice that if $r^{(2)}_0$ belongs to the previous Krylov subspace K_m , then the term $|| (I-P_m)r^{(2)}_0 ||_{A^{-1}}$ in the right hand side of (14) vanishes. The proposition then indicates that in this case the method will provide a good accuracy when α is not too large. In fact the accuracy will be of the same order as that obtained from m steps of the regular conjugate gradient method. Note that if $\alpha=0$ then the term ϵ is zero. As a consequence an extreme case where the new system can be exactly solved by the application of the projection process would be when the two following conditions are fulfilled:

•
$$(I-P_m) r_0^{(2)} = 0$$
, i.e. $r_0^{(2)} \in K_m$

• and $\alpha = 0$, i.e. $r_0^{(2)}$ has no component in v_1 ;

The opposite extreme case is when the projection process leaves the starting approximate solution $x_0^{(2)}$ unchanged. This happens when $P_m r_0^{(2)} = 0$, i.e. when $r_0^{(2)}$ is orthogonal to K_m . In

this case $\alpha = 0$ and the proposition yields $||\bar{r}||_{A^{-1}} = ||r_0^{(2)}||_{A^{-1}}$ which is clearly true since $\bar{z} = x_0^{(2)}$.

More realistic situations arising in practice will lie somewhere between these two extremes. For such general cases the proposition shows that the error consits in a 'small' part ϵ and a 'large' part $|| (I-P_m)r^{(2)}_0 ||_{A^{-1}}$. The 'small' part is usually as small as would be obtained from m 'average' steps of the conjugate algorithm. The 'large' part depends essentially on the new system and can be quite large as compared with ϵ . Perhaps the most interesting and useful such situations arise in time dependent, or more generally parameter dependent poblems, in which the right hand sides $b^{(i)}$, i=1,2,... change very little. Then the system can be expected to be solved relatively accurately because the 'large' term $|| (I-P_m)r_0^{(2)} ||_{A^{-1}}$ becomes small.

When $||(I-P_m) r_0^{(2)}||_{A^{-1}}$ is large, then it is likely that the error in the A^{-1} -norm sense cannot be decreased below $||(I-P)r_0^{(2)}||_{A^{-1}}$ by the projection process (12) alone. This means that some additional refinement must be applied.

4. Refining the Lancsos-Galerkin approximation

Let us start by summarizing the essential of the two stages of the process described in the previous section.

- 1. We have solved the first linear system $Ax^{(1)} = b^{(1)}$ by the Lanczos method and this has provided us with a Krylov subspace K_m of dimension m, an orthonormal basis $V_m = [v_1, v_2, ... v_m]$ of that subspace and a tridiagonal matrix T_m , representing the section of A in K_m , with respect to this basis.
- 2. We are faced with a new system $Ax^{(2)} = b^{(2)}$, for which an initial guess $x_0^{(2)}$ is available. This approximation is improved by use of the Lanczos-Galerkin projection process which yields the approximation:

$$\bar{z} = x_0^{(2)} + V_m T_m^{-1} V_m^T r_0^{(2)}$$

whose residual vector is $\bar{r} = b - A \bar{z}$.

We have at this stage shown only how to improve an initial solution $x_0^{(2)}$ to the second system given the data gathered from the first system by use of a Galerkin projection process on K_m . The accuracy of \bar{z} thus obtained may be far from sufficient as is shown by the comments at the end of the previous section. We are therefore faced with the problem of improving the new approximation \bar{z} . An easy way of achieving this is by a completely new sequence of Lanczos

approximations starting with \bar{z} . However, this does not fully take advantage of the available information, i.e. of the previous Krylov subspace and the representation T_m . A suitable alternative would be one which continues naturally the previous process by constructing a sequence of subspaces containing K_m and of increasing dimension.

One such process was first introduced by Parlett [7] and was later rediscovered by Carnoy and Geradin [1] in a different context. The following algorithm, which will be referred to as the modified Lanczos algorithm, differs only in its presentation from Parlett's algorithm and the algorithm in $\text{cite}\{\text{Carnoy-Geradin}\}$. Its purpose is to compute a sequence of vectors \mathbf{w}_i , i=1,2,... which is orthonormal and also orthogonal to the \mathbf{v}_i 's, i=1,...,m, generated for the first system.

Modified Lanczos Algorithm

1. Start: take
$$\mathbf{w}_1 = \bar{\mathbf{r}}/||\bar{\mathbf{r}}||$$

2. Iterate: For j=1,2,...do

Compute
$$\tilde{\alpha}_j = (Aw_j, w_j)$$

$$\delta_{j} = (A \mathbf{w}_{j}, \mathbf{v}_{m})$$

$$\hat{\mathbf{w}}_{j+1} = A \mathbf{w}_{j} - \tilde{\alpha}_{j} \mathbf{w}_{j} - \overline{\beta}_{j} \mathbf{w}_{j-1} - \delta_{j} \mathbf{v}_{m}$$

$$\overline{\beta}_{j+1} = ||\hat{\mathbf{v}}_{j+1}||$$

$$\mathbf{w}_{j+1} = \hat{\mathbf{w}}_{j+1} / \overline{\beta}_{j+1}$$
(20)

All the difference with the usual Lanczos algorithm is that at each step we now orthogonalize against one more vector, namely the vector $\mathbf{v}_{\mathbf{m}}$. We claim that this simple modification of the Lanczos algorithm, yields a sequence of vectors so that the system $\mathbf{W}_{\mathbf{p}} = \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_{\mathbf{m}}, \mathbf{w}_1, ... \mathbf{w}_{\mathbf{p}}\}$ is orthonormal. This is an important property since it will allow us to realize in a simple way, as will be seen shortly, the Galerkin process onto the span of $\mathbf{W}_{\mathbf{p}}$.

Proposition 2: Suppose that p steps of the Modified Lanczos algorithm are feasible. Then the sequence $v_1, v_g, ..., v_m, w_1, w_g, ..., w_p$, forms an orthonormal sequence of vectors.

Proof: Since $\{v_j\}_{j=1,m}$ is an orthonormal system, we must prove that for j=1,2,... we have:

- 1. w_i is orthogonal to the v_i 's i=1,.m
- 2. w_i is orthogonal to the previous w_i 's, i=1,2,...j-1.

The proof in by induction. Clearly the above property is true for j=1, because w_1 is equal to \bar{r} apart from a multiplicative constant and \bar{r} is known to be orthogonal to the subspace K_m by the Galerkin condition. Suppose that the propoerty is true for j and let us prove that it is true for j+1, i.e. that

$$(\mathbf{w}_{i+1}, \mathbf{v}_i) = 0, i=1,2...\mathbf{m}$$
 (21)

$$(\mathbf{w}_{i+1}, \mathbf{w}_i) = 0, i=1,2,...j.$$
 (22)

Consider (21) first. By construction, $(\mathbf{w}_{i+1}, \mathbf{v}_{m}) = 0$, so we can restrict ourselves to the case i < m.

$$(\mathbf{w}_{i+1}, \mathbf{v}_i) = (\overline{\beta}_{i+1})^{-1} \left[(A\mathbf{w}_j, \mathbf{v}_i) - \overline{\alpha}_i (\mathbf{w}_j, \mathbf{v}_i) - \overline{\beta}_i (\mathbf{w}_{j-1}, \mathbf{v}_i) - \delta_i (\mathbf{v}_m, \mathbf{v}_i) \right]$$

By the induction hypothesis and because $\{v_i\}_{i=1,m}$ is orthogonal, the terms (w_j, v_i) , (w_{j-1}, v_i) and (v_m, v_i) on the right hand side all vanish. The remaining term (Aw_j, v_i) can be expanded as follows:

$$\begin{aligned} (A \mathbf{w}_{j}, \mathbf{v}_{i}) &= (\mathbf{w}_{j}, A \mathbf{v}_{i}) = (\mathbf{w}_{j}, \beta_{i+1} \mathbf{v}_{i+1} + \alpha_{i} \mathbf{v}_{i} + \beta_{i} \mathbf{v}_{i-1}) \\ &= \beta_{i+1} (\mathbf{w}_{i}, \mathbf{v}_{i+1}) + \alpha_{i} (\mathbf{w}_{i}, \mathbf{v}_{i}) + \beta_{i} (\mathbf{w}_{i}, \mathbf{v}_{i-1}) \end{aligned}$$

Using again the induction hypothesis, we see that all these terms are in turn equal to zero. This completes the proof of (21).

Now consider (22).

$$(\mathbf{w}_{j+1}, \mathbf{w}_i) = [\overline{\beta}_{j+1}]^{-1} [(\mathbf{A}\mathbf{w}_j, \mathbf{w}_i) - \overline{\alpha}_j(\mathbf{w}_j, \mathbf{w}_i) - \overline{\beta}_j(\mathbf{w}_{j-1}, \mathbf{w}_i) - \delta_j(\mathbf{v}_m, \mathbf{w}_i)]$$

Assume first that i < j - 1. By the induction hypothesis we obviously have

$$(\mathbf{w}_{i}, \mathbf{w}_{i}) = (\mathbf{w}_{i-1}, \mathbf{w}_{i}) = (\mathbf{v}_{m}, \mathbf{w}_{i}) = 0.$$

Proceeding as before, we expand the remaining term (Awi,wi) as follows:

$$\begin{split} (\mathbf{A}\mathbf{w}_{j}, &\mathbf{w}_{i}) = (\mathbf{w}_{j}, \mathbf{A}\mathbf{w}_{i}) = (\mathbf{w}_{j}, \overline{\beta}_{i+1}\mathbf{w}_{i+1} + \overline{\alpha}_{i}\mathbf{w}_{i} + \overline{\beta}_{i}\mathbf{w}_{i-1} + \delta_{i}\mathbf{v}_{m}) \\ &= \overline{\beta}_{i+1}(\mathbf{w}_{j}, \mathbf{w}_{i+1}) + \overline{\alpha}_{i}(\mathbf{w}_{j}, \mathbf{w}_{i}) + \overline{\beta}_{i}(\mathbf{w}_{j}, \mathbf{w}_{i-1}) + \delta_{i}(\mathbf{w}_{j}, \mathbf{v}_{m}) \end{split}$$

which, by a final application of the induction hypothesis shows that $(Aw_j, w_i)=0$. Hence $(w_{j+1}, w_i)=0$, for i < j-1. For i=j and i=j-1, the scalars $\bar{\alpha}_j$, $\overline{\beta}_j$, and δ_j have been precisely chosen so that the property is true. This completes the proof.

Consider the subspace spanned by the orthonormal system $W_p = [v_1, v_2, ..., v_m, w_1, ..., w_p]$ which we will denote by $K_{m,p}$. Note that $K_{m,p}$ is no longer a Krylov subspace but, as will be seen shortly, the case p=m is of particular importance. The matrix representation $W_p^T A W_p$ of the section of

A in the subspace $K_{m,p}$, with respect to the basis W_p is the $(m+p) \times (m+p)$ matrix:

$$T_{\bullet,p} = \begin{bmatrix} \alpha_1 & \beta_2 \\ \beta_2 & \alpha_2 & \beta_3 \\ & \beta_3 & \alpha_3 \\ & & \vdots \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

Hence the new approximate solution obtained at step p of the projection process onto the subspace $K_{m,p}$ is given by:

$$z_{p} = \bar{z} + W_{p} T_{m,p}^{-1} W_{p}^{T} \bar{r}$$

Noticing that $W_p^T \bar{i} = W_p^T ||\bar{z}|| \mathbf{w}_1$, this simplifies into:

$$z_{p} = \bar{z} + ||\bar{r}|| W_{p} T_{m,p}^{-1} e_{m+1}$$

where e_{m+1} is the vector of length m+p whose components are zero except the $(m+1)^{st}$ which is equal to 1. Once the augmented tridiagonal system $T_{m,p}$ s = e_{m+1} is solved, the linear combination W_p s of the vectors \mathbf{v}_i and \mathbf{w}_i should be formed and added to $\bar{\mathbf{z}}$. The whole set of vectors W_p must therefore be kept in storage.

It is important to interpret the method outlined above, in order to compare its rate of convergence with that of the regular Lanczos process. We will establish the following result for the particular case where p=m.

Proposition 3: When p=m, the modified Lanczos process is equivalent to m steps of the block Lanczos method with block dimension of 2, with starting block consisting of the vectors v, and w,.

Proof: The proof amounts to showing that the two methods realize the Galerkin process on the same subspace.

For the block Lanczos method [5, 14, 12], the subspace is simply span $\{S_1,AS_1,...A^{m-1}S_1\}$ where $S_1 = \{v_1,w_1\}$.

The modified Lanczos algorithm is a projection process onto the subspace

 $v_1, v_2, ..., v_m, w_1, w_2, ..., w_m$. It is a simple exercise on proofs by induction to show from the gorithm that the v_i 's and w_i 's are linear combinations of the vectors $A^k v_1$ and $A^j w_1$, $\leq k, j \leq m-1$ and vice-versa. Thus the two subspaces are identical and the proof is complete.

The proposition asserts that there are two ways of realizing the block Lanczos method. One is no regular algorithm in either its block form [14] or its banded form [8], and is suitable for the use when the linear systems are available simultneously. The other way is the modified Lanczos ignithm which is more suitable when the right hand sides are not available simultaneously, i.e. hen the right hand side $b^{(2)}$ depends on the solution $x^{(1)}$ of the first system.

The rate of convergence of the block Lanczos algorithm for solving linear systems has been sudied in [5, 11] and we will not report the results here. It suffices to say that, not surprisingly, he bounds on the rate of convergence of the block method are superior to those of the single ector method. We should point out however that our experience reveals that when only one ystem is to be solved it is not in general effective to use a block method as a means of ccelerating the convergence [11].

To summarize, the modified Lanczos method has the advantage of the rapid convergence of he block Lanczos method without the drawback of requiring that the second right hand side be vailable at the same time as the first.

. Practical Considerations

One important feature of both the Lanczos-Galerkin Process and the modified Lannczos rocess is that we must save a large number of vectors in some secondary storage. This may seem impractical at first but there are numerous reasons why it is not always so:

- Once a vector has been computed it is not needed until the convergence of the process is reached. There exists a simple formula for evaluating the residual norm of the solution without even having to compute the solution [7, 10] thus allowing to determine when to stop.
- There are supercomputer systems with very fast auxiliary memories, e.g. the Cray-XMP with Solid-state Storage Device (SSD).
- In many cases the dominant cost is the matrix by vector product and therefore the priority is to economize on the number of matrix by vector multiplications. The Lanczos-Galerkin process of section 3 requires only one matrix-vector product (for

computing the initial residual $r_0^{(2)}$).

The Lanczos-Galerkin process was successfully used in the context of stiff ODE's [3]. In some ODE problems the cost of a matrix by vector multiplication can be extremely high and the Lanczos-Galerkin process becomes very attractive.

In the context of symmetric generalized eigenvalue problems, a technique similar to the one described in the previous section has recently been presented by Carnoy and Geradin [1], who report some interesting numerical results.

It seems important that the vectors $\mathbf{v_i}$'s that must be saved from the first linear system, be orthogonal because the Lanczos-Galerkin process is essentially based on the orthogonality of these vectors. The Selective Orthogonalization [7] and the Partial Orthogonalization [13] methods can both be extended to the modified Lanczos method and are attractive alternatives to the more expensive full reorthogonalization schemes. Simon [13] has shown that any partial reorthogonalization that guaranties semi-orthogonality, i.e. orthogonality within the square root of the machine accuracy ϵ , will also deliver an approximate solution vector that is within $\sqrt{\epsilon}$ of the ideal solution vector from the Krylov subspace.

Although not explicitly mentioned, it is clear that the techniques of the previous two sections can easily be extended to systems with more than two right hand sides. The resulting algorithms are straightforward and so is the theory.

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